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(FILE 'HOME' ENTERED AT 08:17:54 ON 27 SEP 1999)

INDEX '1MOBILITY, 2MOBILITY, ADISALERTS, AEROSPACE, AGRICOLA, AIDSLINE,
ALUMINIUM, ANABSTR, APILIT, APIPAT, AQUASCI, BIBLIODATA, BIOBUSINESS,
BIOCOMMERCE, BIOSIS, BIOTECHABS, BIOTECHDS, BLLDB, CABA, CANCERLIT,
CAPLUS, CBNB, CEABA, CEN, CERAB, CHEMSAFE, ...' ENTERED AT 08:18:06 ON 27
SEP 1999
L1 SEA (NMR OR NOESY OR NUCLEAR(W)MAGNETIC(W)RESONANCE) AND (THREE
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2 FILE AEROSPACE
106 FILE AGRICOLA
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L1 QUE (NMR OR NOESY OR NUCLEAR(W) MAGNETIC(W) RESONANCE) AND (THR

FILE 'AGRICOLA, MEDLINE, BIOSIS, CAPLUS, EMBASE, ENERGY, LIFESCI, JICST-EPLUS, TOXLINE' ENTERED AT 08:36:39 ON 27 SEP 1999
L2 2072 S L1 AND (FUNCTION OR ACTIVITY)
L3 87 S L2 AND (ALGORITHM#)
L4 40 DUPLICATE REMOVE L3 (47 DUPLICATES REMOVED)
L5 2 S L2 AND (HIGH(W)THROUGHPUT)

=> s l2 and pars?

L6 1 L2 AND PARS?

=> d bib ab

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 1999 ACS
AN 1999:146268 CAPLUS
TI ***Protein*** ***NMR*** and the human proteome project
AU Montelione, Gaetano T.
CS Center for Advanced Biotechnology Medicine and Department of Molecular Biology and Biochemistry, Rutgers University, Piscataway, NJ, 08854, USA
SO Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25 (1999), POLY-232 Publisher: American Chemical Society, Washington, D. C.
CODEN: 67GHA6
DT Conference; Meeting Abstract
LA English
AB Genome sequencing projects are rapidly identifying all of the genes in several organisms. The products of these genes are widely recognized as the next generation of therapeutics and targets for the development of pharmaceuticals. While identification of these genes is proceeding quickly, elucidation of their ***three*** ***dimensional*** (3D) structures and biochem. functions lags far behind. In some cases, knowledge of 3D structures of ***proteins*** can provide important insights into structural homol. that is not easily recognized by sequence alignment comparisons. Thus, anal. of a ***protein*** 's 3D structure by ***NMR*** or X-ray crystallog. prior to characterization of the ***protein*** 's biochem. ***function*** can sometimes provide key information regarding ***protein*** fold class, locations and clustering of conserved residues, and surface electrostatic field distributions. This information can be used to develop hypotheses regarding potential biochem. functions, and the resulting limited set of putative biochem. functions tested by appropriate biochem. assays. ***NMR*** chem. shift assignments and soln. structures of ***proteins*** also provide the basis for epitope-mapping, mol. dynamics, and SAR studies, and set the stage for subsequent drug development using combinatorial and/or rational design methods. We are developing technologies that will significantly accelerate the process of structure detn. by ***NMR*** . These include bioinformatics methods for ***parsing*** novel genes into domain encoding regions, high-level "multiplexed" ***protein*** expression systems, and ***NMR*** pulse sequences, data collection methods, and expert-system software for automated anal. of ***protein*** resonance assignments and 3D structures. These technologies and the resulting exptl. data are being organized and integrated using relational databases. The goal of this work is to develop a "high-throughput" process for structural anal. of novel gene products on a genomic scale. In a pilot project, these techniques are being applied to clusters of orthologous genes coding for ***proteins*** of unknown structure and ***function*** , with the aim of testing the hypothesis that 3D structural anal. can sometimes provide useful and important clues regarding the biochem. functions of orphan gene products. The relationship of our effort and the emerging international interest in a large-scale Human Proteome Project will be discussed.

=> s l2 and multiplex?

L7 1 L2 AND MULTIPLEX?

=> s l2 and (structure# (4a) function?)

6 FILES SEARCHED...
L8 428 L2 AND (STRUCTURE# (4A) FUNCTION?)

=> duplicate remove l8

DUPLICATE PREFERENCE IS 'AGRICOLA, MEDLINE, BIOSIS, CAPLUS, EMBASE, ENERGY, LIFESCI, JICST-EPLUS, TOXLINE'
KEEP DUPLICATES FROM MORE THAN ONE FILE? Y/(N):n

PROCESSING COMPLETED FOR L8
L9 189 DUPLICATE REMOVE L8 (239 DUPLICATES REMOVED)

=> d 1-189 ti

L9 ANSWER 1 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Compositions and methods to inhibit formation of the C5B-9 complex of complement

L9 ANSWER 2 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Linking gene sequence to gene ***function*** by ***three*** - ***dimensional*** ***protein*** ***structure*** determination using ***NMR***

L9 ANSWER 3 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI The AcbC ***protein*** from Actinoplanes species is a C7-cyclitol synthase related to 3-dehydroquinate synthases and is involved in the biosynthesis of the alpha-glucosidase inhibitor acarbose.

L9 ANSWER 4 OF 189 MEDLINE
TI Effects of substitutions of lysine and aspartic acid for asparagine at beta 108 and of tryptophan for valine at alpha 96 on the structural and functional properties of human normal adult hemoglobin: roles of alpha 1 beta 1 and alpha 1 beta 2 subunit interfaces in the cooperative oxygenation process.

L9 ANSWER 5 OF 189 MEDLINE DUPLICATE 1
TI ***NMR*** ***structure*** and ***functional*** studies of the Mu repressor DNA-binding domain.

L9 ANSWER 6 OF 189 MEDLINE DUPLICATE 2
TI Disulfide bridges in interleukin-8 probed using non-natural disulfide analogues: dissociation of roles in ***structure*** from ***function*** .

L9 ANSWER 7 OF 189 MEDLINE DUPLICATE 3
TI Solution structure of the chicken cysteine-rich ***protein*** , CRP1, a double-LIM ***protein*** implicated in muscle differentiation.

L9 ANSWER 8 OF 189 MEDLINE DUPLICATE 4
TI Structure and dynamics of ***peptide*** -amphiphiles incorporating triple-helical proteinlike molecular architecture.

L9 ANSWER 9 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 5
TI Comparative modeling of amoebapores and granulysin based on the NK-lysin ***structure*** . Structural and ***functional*** implications

L9 ANSWER 10 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 6
TI Autoprocessing of HIV-1 protease is tightly coupled to ***protein*** folding

L9 ANSWER 11 OF 189 MEDLINE DUPLICATE 7
TI The solution structure of a superpotent B-chain-shortened single-replacement insulin analogue.

L9 ANSWER 12 OF 189 MEDLINE DUPLICATE 8
TI Solution structure of toxin 2 from centruroides noxius Hoffmann, a beta-scorpion neurotoxin acting on sodium channels.

L9 ANSWER 13 OF 189 MEDLINE DUPLICATE 9
TI Chimeras of human extracellular and intracellular superoxide dismutases. Analysis of ***structure*** and ***function*** of the individual domains.

L9 ANSWER 14 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE
TI Effective computational strategies for determining structures of carcinogen-damaged DNA.

L9 ANSWER 15 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Motional dynamics of the catalytic loop in OMP synthase.

L9 ANSWER 16 OF 189 MEDLINE DUPLICATE 10
TI Smoluchowski dynamics of the vnd/NK-2 homeodomain from Drosophila melanogaster: first-order mode-coupling approximation.

L9 ANSWER 17 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Protein*** ***NMR*** and the human proteome project

L9 ANSWER 18 OF 189 MEDLINE DUPLICATE 11
TI Secondary structure of the C-terminal DNA-binding domain of the transcriptional activator NifA from Klebsiella pneumoniae: spectroscopic analyses.

L9 ANSWER 19 OF 189 MEDLINE DUPLICATE 12
TI Purification and characterization of a plant antimicrobial ***peptide*** expressed in Escherichia coli.

L9 ANSWER 20 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Characterization of ***protein*** -glycolipid recognition at the membrane bilayer.

L9 ANSWER 21 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 13
TI Acylation-stimulating ***protein*** (ASP): ***structure*** - ***function*** determinants of cell surface binding and triacylglycerol synthetic ***activity***

L9 ANSWER 22 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Structural biology of HIV.

L9 ANSWER 23 OF 189 TOXLINE
TI MUTAGENESIS AND REPAIR OF DNA.

L9 ANSWER 24 OF 189 TOXLINE
TI ISOTOPIC PROBES OF ENZYMATIC REACTION MECHANISMS.

L9 ANSWER 25 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Characterization of antibacterial COOH-terminal proenkephalin-A-derived ***peptides*** (PEAP) in infectious fluids. Importance of enkelytin, the antibacterial PEAP209-237 secreted by stimulated chromaffin cells

L9 ANSWER 26 OF 189 MEDLINE DUPLICATE 14
TI Yeast transcript elongation factor (TFIIS), ***structure*** and ***function*** . I: ***NMR*** structural analysis of the minimal transcriptionally active region.

L9 ANSWER 27 OF 189 MEDLINE DUPLICATE 15
TI High-resolution solution ***NMR*** structure of the minimal active domain of the human immunodeficiency virus type-2 nucleocapsid ***protein*** .

L9 ANSWER 28 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Functional requirements for specific ligand recognition by a biotin-binding rna pseudoknot.

L9 ANSWER 29 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI The ***NMR*** structure of Escherichia coli ribosomal ***protein*** L25 shows homology to general stress ***proteins*** and glutaminyl-tRNA synthetases.

L9 ANSWER 30 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Conformational analysis and automated receptor docking of selective arylacetamide-based .kappa.-opioid agonists.

L9 ANSWER 31 OF 189 AGRICOLA DUPLICATE 16
TI Micelle stability: kappa-casein ***structure*** and ***function*** .

L9 ANSWER 32 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Solution structure of the SH3 domain from Bruton's tyrosine kinase.

L9 ANSWER 33 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Structure of human cyclin-dependent kinase inhibitor p19INK4d: comparison to known ankyrin-repeat-containing structures and implications for the dysfunction of tumor suppressor p16INK4a

L9 ANSWER 34 OF 189 MEDLINE DUPLICATE 17
TI Method for prediction of ***protein*** ***function*** from sequence using the sequence-to- ***structure*** -to- ***function*** paradigm with application to glutaredoxins/thioredoxins and T1 ribonucleases.

L9 ANSWER 35 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Solution structure of Compstatin, a potent complement inhibitor.

L9 ANSWER 36 OF 189 MEDLINE DUPLICATE 18
TI The relationship between insulin bioactivity and structure in the NH2-terminal A-chain helix.

L9 ANSWER 37 OF 189 MEDLINE
TI Recent trends in ***protein*** structural studies.

L9 ANSWER 38 OF 189 MEDLINE DUPLICATE 19
TI ***Structure*** - ***function*** analysis of a series of glucagon-like ***peptide*** -1 analogs.

L9 ANSWER 39 OF 189 MEDLINE DUPLICATE 20
TI The ***structure*** and ***function*** of HPr.

L9 ANSWER 40 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI The development of ***NMR*** methods to study ***protein*** structure and dynamics

L9 ANSWER 41 OF 189 MEDLINE DUPLICATE 21
TI Non-homology knowledge-based prediction of the papain prosegment folding pattern: a description of plausible folding and activation mechanisms.

L9 ANSWER 42 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Probing the structure of the human Ca2+- and Zn2+-binding ***protein*** S100A3: Spectroscopic investigations of its transition metal ion complexes, and ***three*** - ***dimensional*** structural model.

L9 ANSWER 43 OF 189 MEDLINE DUPLICATE 22
TI Energy strain in ***three*** - ***dimensional*** ***protein*** structures.

L9 ANSWER 44 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI The atypical serine proteases of the complement system.

L9 ANSWER 45 OF 189 MEDLINE DUPLICATE 23
TI ***Structure*** - ***function*** relationships of antimicrobial ***peptides*** .

L9 ANSWER 46 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

TI ***NMR*** analysis of a potent decapeptide agonist of human C5a anaphylatoxin.

L9 ANSWER 47 OF 189 MEDLINE DUPLICATE 24
TI Sequence-specific 1H assignment and secondary structure of the bacteriocin AS-48 cyclic ***peptide*** .

L9 ANSWER 48 OF 189 MEDLINE DUPLICATE 25
TI Structure and properties of surfactant ***protein*** C.

L9 ANSWER 49 OF 189 JICST-EPlus COPYRIGHT 1999 JST
TI ***Three*** - ***dimensional*** Structure of .DELTA.-conotoxin TxVIA.

L9 ANSWER 50 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Insights into the structure of hepatocyte growth factor/scatter factor (HGF/SF) and implications for receptor activation

L9 ANSWER 51 OF 189 MEDLINE DUPLICATE 26
TI Mini-proinsulin and mini-IGF-I: homologous ***protein*** sequences encoding non-homologous structures.

L9 ANSWER 52 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 27
TI ***Structure*** and ***function*** of ***peptide*** and ***protein*** toxins from marine organisms.

L9 ANSWER 53 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Metal coordination of azurin in the unfolded state.

L9 ANSWER 54 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Accessibility of selenomethionine ***proteins*** by total chemical synthesis: Structural studies of human herpesvirus-8 MIP-II.

L9 ANSWER 55 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Structure*** and ***function*** of charybdotoxin are not affected by substitution of an interior cystine with two alpha.-amino-n-butyric acid (Aba) residues

L9 ANSWER 56 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 28
TI The role of leucine residues in the ***structure*** and ***function*** of a leucine zipper ***peptide*** inhibitor of paramyxovirus (NDV) fusion

L9 ANSWER 57 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Synthetic RNA modification and crosslinking approaches towards the structure of the hairpin ribozyme and the HIV-1 Tat ***protein*** interaction with TAR RNA

L9 ANSWER 58 OF 189 JICST-EPlus COPYRIGHT 1999 JST
TI Modern ***NMR*** Spectroscopy and X-ray Crystallography: a different approach to study the ***structure*** and its ***function*** of a ***protein*** .

L9 ANSWER 59 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI ***Three*** - ***dimensional*** ***structure*** of lactoferrin: Implications for ***function*** , including comparisons with transferrin.

L9 ANSWER 60 OF 189 TOXLINE
TI MUTAGENESIS AND REPAIR OF DNA.

L9 ANSWER 61 OF 189 TOXLINE
TI ISOTOPIC PROBES OF ENZYMATIC REACTION MECHANISMS.

L9 ANSWER 62 OF 189 MEDLINE DUPLICATE 29
TI Site-directed mutagenesis and characterization of uracil-DNA glycosylase inhibitor ***protein*** . Role of specific carboxylic amino acids in complex formation with Escherichia coli uracil-DNA glycosylase.

L9 ANSWER 63 OF 189 MEDLINE DUPLICATE 30
TI Comparison of the hemolytic ***activity*** and solution structures of two snake venom cardiotoxin analogues which only differ in their N-terminal amino acid.

L9 ANSWER 64 OF 189 LIFESCI COPYRIGHT 1999 CSA
TI Comparison of the hemolytic ***activity*** and solution structures of two snake venom cardiotoxin analogues which only differ in their N-terminal amino acid

L9 ANSWER 65 OF 189 MEDLINE DUPLICATE 31
TI Structural mimicry of a native ***protein*** by a minimized binding domain.

L9 ANSWER 66 OF 189 MEDLINE DUPLICATE 32
TI Structure of the C-terminal fragment 300-320 of the rat angiotensin II AT1A receptor and its relevance with respect to G- ***protein*** coupling.

L9 ANSWER 67 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 33
TI ***Structure*** and ***Function*** of an Aromatic Ensemble That Restricts the Dynamics of the Hydrophobic Core of a Designed Helix-Loop-Helix Dimer

L9 ANSWER 68 OF 189 MEDLINE DUPLICATE 34
TI Solution structure of the Mu end DNA-binding ibeta subdomain of phage Mu transposase: modular DNA recognition by two tethered domains.

L9 ANSWER 69 OF 189 MEDLINE DUPLICATE 35
TI Solution ***structure*** and basis for ***functional*** ***activity*** of stromal cell-derived factor-1; dissociation of CXCR4 activation from binding and inhibition of HIV-1.

L9 ANSWER 70 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI On the convergent evolution of animal toxins. Conservation of a diad of functional residues in potassium channel-blocking toxins with unrelated structures

L9 ANSWER 71 OF 189 MEDLINE DUPLICATE 36
TI TESS: a geometric hashing algorithm for deriving 3D coordinate templates for searching structural databases. Application to enzyme active sites.

L9 ANSWER 72 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Cloning, purification, and preliminary characterization by circular dichroism and ***NMR*** of a carboxyl-terminal domain of the bacteriophage P22 scaffolding ***protein***

L9 ANSWER 73 OF 189 MEDLINE DUPLICATE 37
TI ***Structure*** - ***function*** relationships of cellular retinoic acid-binding ***proteins*** . Quantitative analysis of the ligand binding properties of the wild-type ***proteins*** and site-directed mutants.

L9 ANSWER 74 OF 189 MEDLINE DUPLICATE 38
TI Assessment by 1H ***NMR*** spectroscopy of the structural behaviour of human parathyroid-hormone-related ***protein*** (1-34) and its close relationship with the N-terminal fragments of human parathyroid hormone in solution.

L9 ANSWER 75 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI The collagen triple-helix structure.

L9 ANSWER 76 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Snake venom cardiotoxins- ***structure*** , dynamics, ***function*** and folding.

L9 ANSWER 77 OF 189 MEDLINE DUPLICATE 39
TI The second Kunitz domain of human tissue factor pathway inhibitor: cloning, structure determination and interaction with factor Xa.

L9 ANSWER 78 OF 189 MEDLINE DUPLICATE 40
TI Refined solution structure of the anti-mammal and anti-insect Lqq!!! scorpion toxin: comparison with other scorpion toxins.

L9 ANSWER 79 OF 189 MEDLINE DUPLICATE 41
TI Solution structure of a type 2 module from fibronectin: implications for the ***structure*** and ***function*** of the gelatin-binding domain.

L9 ANSWER 80 OF 189 MEDLINE DUPLICATE 42
TI The pH-dependent ***tertiary*** ***structure*** of a designed helix-loop-helix dimer.

L9 ANSWER 81 OF 189 MEDLINE DUPLICATE 43
TI Analysis of a ***peptide*** inhibitor of paramyxovirus (NDV) fusion using biological assays, ***NMR*** , and molecular modeling.

L9 ANSWER 82 OF 189 AGRICOLA DUPLICATE 44
TI Solution structure of Lqh-8/6, a toxin-like ***peptide*** from a scorption venom. Structural heterogeneity induced by proline cis/trans isomerization.

L9 ANSWER 83 OF 189 LIFESCI COPYRIGHT 1999 CSA
TI Higher order structures of coxsackievirus B 5' nontranslated region RNA

L9 ANSWER 84 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Amylin, calcitonin gene-related ***peptide*** , calcitonin, and adrenomedullin: a ***peptide*** superfamily

L9 ANSWER 85 OF 189 MEDLINE
TI Endo-beta-1,4-xylanase families: differences in catalytic properties.

L9 ANSWER 86 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Three*** - ***dimensional*** structure and receptor-recognition sites of bombyxin-II, an insulin-like brain-secretory ***peptide*** of the silkmoth

L9 ANSWER 87 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Alterations in chemical shifts and exchange broadening upon ***peptide*** boronic acid inhibitor binding to alpha-lytic protease.

L9 ANSWER 88 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI ***NMR*** -based ***structure*** - ***function*** relation of N-type inactivation in K-v-type K+ channels.

L9 ANSWER 89 OF 189 AGRICOLA DUPLICATE 45
TI ***NMR*** methods for the study of ***protein*** structure and dynamics.

L9 ANSWER 90 OF 189 AGRICOLA DUPLICATE 46
TI 1H ***NMR*** assignment and global fold of napin BnIb, a representative 2S albumin seed ***protein*** .

L9 ANSWER 91 OF 189 MEDLINE DUPLICATE 47
TI ***Three*** - ***dimensional*** solution structure of mu-conotoxin GIIIB, a specific blocker of skeletal muscle sodium channels.

L9 ANSWER 92 OF 189 MEDLINE DUPLICATE 48
TI The cytoplasmic fragment of the aspartate receptor displays globally dynamic behavior.

L9 ANSWER 93 OF 189 MEDLINE DUPLICATE 49
TI Circularly permuted dihydrofolate reductase possesses all the properties of the molten globule state, but can resume ***functional*** ***tertiary*** ***structure*** by interaction with its ligands.

L9 ANSWER 94 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 50
TI ***Tertiary*** ***structure*** and ***functional*** sites of bombyxin, an insect insulin-like ***peptide*** . Comparison with those of insulin

L9 ANSWER 95 OF 189 MEDLINE DUPLICATE 51
TI 1H and 15N ***nuclear*** ***magnetic*** ***resonance*** assignment and secondary structure of the cytotoxic ribonuclease alpha-Sarcin.

L9 ANSWER 96 OF 189 MEDLINE DUPLICATE 52
TI What ***function*** for human lithostathine?: structural investigations by ***three*** - ***dimensional*** structure modeling and high-resolution ***NMR*** spectroscopy.

L9 ANSWER 97 OF 189 MEDLINE DUPLICATE 53
TI Computer modeling of 3D structures of cytochrome P450s.

L9 ANSWER 98 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Structure*** - ***function*** relationship of adenylate kinase: Glu-101 in AMP specificity

L9 ANSWER 99 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Solution structure of protegrin-1, a broad-spectrum antimicrobial ***peptide*** from porcine leukocytes.

L9 ANSWER 100 OF 189 MEDLINE
TI Domain organizations of modular extracellular matrix ***proteins*** and their evolution.

L9 ANSWER 101 OF 189 MEDLINE DUPLICATE 54
TI ***Structure*** - ***function*** relationships of the complement regulatory ***protein*** , CD59.

L9 ANSWER 102 OF 189 MEDLINE
TI Synthesis and conformational analysis by 1H ***NMR*** and restrained molecular dynamics simulations of the cyclic decapeptide [Ser-Tyr-Ser-Met-Glu-His-Phe-Arg-Trp-Gly].

L9 ANSWER 103 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI High frequency of mutational changes during the cloning of a human centromeric repeat

L9 ANSWER 104 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI ***NMR*** structure of HMfB from the hyperthermophile, Methanothermus fervidus, confirms that this archaeal ***protein*** is a histone.

L9 ANSWER 105 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 55
TI 3-D Reconstructions from ice-embedded and negatively stained biomacromolecular assemblies: A critical comparison.

L9 ANSWER 106 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 56
TI Modern ***NMR*** spectroscopy and x-ray crystallography. Different approaches to study the ***structure*** and its ***function*** of a ***protein***

L9 ANSWER 107 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Structure of a cyclic ***peptide*** with a catalytic triad, determined by computer simulation and ***NMR*** spectroscopy

L9 ANSWER 108 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Structure*** and ***function*** of the single-stranded DNA binding ***proteins*** of the filamentous bacteriophages M13 and Pf3. ***NMR*** studies

L9 ANSWER 109 OF 189 TOXLINE
TI BIOLOGICAL CONSEQUENCES OF SITE-SPECIFIC DAMAGE TO DNA.

L9 ANSWER 110 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Reactive-Site Hydrolyzed Cucurbita maxima Trypsin Inhibitor-V: ***Function*** , Thermodynamic Stability, and ***NMR*** Solution Structure

L9 ANSWER 111 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Catalytic domain of human immunodeficiency virus type 1 integrase: Identification of a soluble mutant by systematic replacement of hydrophobic residues.

L9 ANSWER 112 OF 189 MEDLINE DUPLICATE 57
TI Biological and structural characterization of a Ras transforming mutation at the phenylalanine-156 residue, which is conserved in all members of the Ras superfamily.

L9 ANSWER 113 OF 189 MEDLINE DUPLICATE 58
TI The zinc coordination site of the bacteriophage Mu translational activator ***protein*** , Com.

L9 ANSWER 114 OF 189 MEDLINE DUPLICATE 59
TI ***Structure*** - ***function*** studies of mEGF: probing the type I beta-turn between residues 25 and 26.

L9 ANSWER 115 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Determination of the structure of exochelin MN, the extracellular siderophore from Mycobacterium neoaurum

L9 ANSWER 116 OF 189 MEDLINE DUPLICATE 60
TI Structures of bacterial immunoglobulin-binding domains and their complexes with immunoglobulins.

L9 ANSWER 117 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Determination of the solution structure of apo calbindin D9k by ***NMR*** spectroscopy

L9 ANSWER 118 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Three*** ***dimensional*** structure of .omega.-agatoxin IVA determined by 1H- ***NMR***

L9 ANSWER 119 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Mass spectrometric approaches to the characterization of tertiary and supramolecular structures of biomacromolecules

L9 ANSWER 120 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI ***NMR*** : This other method for ***protein*** and nucleic acid structure determination.

L9 ANSWER 121 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Water molecules within and around ***proteins*** .

L9 ANSWER 122 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Solution structure of the DNA binding domain of a nucleoid-associated ***protein*** , H-NS, from Escherichia coli.

L9 ANSWER 123 OF 189 MEDLINE DUPLICATE 61
TI Solution ***structure*** and ***function*** in trifluoroethanol of PP-50, an ATP-binding ***peptide*** from F1ATPase.

L9 ANSWER 124 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Structure of the presynaptic (Y-2) receptor-specific neuropeptide Y analog ANA-NPY.

L9 ANSWER 125 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 62
TI ***Structure*** and ***function*** of ***protein*** modules

L9 ANSWER 126 OF 189 MEDLINE DUPLICATE 63
TI ***Three*** - ***dimensional*** structures of alpha and beta chemokines.

L9 ANSWER 127 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE
TI Structural studies on leukaemia inhibitory factor.

L9 ANSWER 128 OF 189 TOXLINE
TI BIOLOGICAL CONSEQUENCES OF SITE-SPECIFIC DAMAGE TO DNA.

L9 ANSWER 129 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI ***Function*** and ***three*** - ***dimensional*** ***structure*** of ***proteins*** using ***nuclear*** ***magnetic*** ***resonance*** spectroscopy.

L9 ANSWER 130 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI Sialyl Lewis X mimics derived from a pharmacophore search are selectin inhibitors with anti-inflammatory ***activity*** .

L9 ANSWER 131 OF 189 MEDLINE DUPLICATE 64
TI Receptor-binding affinities of human epidermal growth factor variants

having unnatural amino acid residues in position 23.

L9 ANSWER 132 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI DNA binding and bending properties of the post-meiotically expressed Sry-related ***protein*** Sox-5.

L9 ANSWER 133 OF 189 MEDLINE DUPLICATE 65
TI Site-directed mutagenesis in hemoglobin: functional and structural role of the penultimate tyrosine in the alpha subunit.

L9 ANSWER 134 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Three*** ***dimensional*** structures of SH2 and SH3 domains

L9 ANSWER 135 OF 189 MEDLINE
TI Cardiotoxin III from the Taiwan cobra (Naja naja atra). Determination of structure in solution and comparison with short neurotoxins.

L9 ANSWER 136 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Solution structure of a specific DNA complex of the Myb DNA-binding domain with cooperative recognition helices.

L9 ANSWER 137 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Solution structure of a gamma-carboxyglutamic acid-rich ***peptide*** of factor IX by two-dimensional ***nuclear*** ***magnetic*** ***resonance*** spectroscopy.

L9 ANSWER 138 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Solution structure of a cysteine rich domain of rat ***protein*** kinase C.

L9 ANSWER 139 OF 189 MEDLINE
TI Empirical studies of ***protein*** secondary structure by vibrational circular dichroism and related techniques. Alpha-lactalbumin and lysozyme as examples.

L9 ANSWER 140 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Stabilized ***NMR*** structure of the hypercalcemia of malignancy ***peptide*** PTHrP(Ala-26)(1-34) amide.

L9 ANSWER 141 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Structure of the C3HC4 domain by 1H- ***nuclear*** ***magnetic*** ***resonance*** spectroscopy. A new structural class of zinc-finger

L9 ANSWER 142 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Structure of a soluble, glycosylated form of the human complement regulatory ***protein*** CD59.

L9 ANSWER 143 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI ***Structure*** and ***function*** of IRES, the noncoding mRNA sequences regulating synthesis of ferritin, transferrin receptor and (erythroid) 5- aminolevulinate synthase.

L9 ANSWER 144 OF 189 MEDLINE DUPLICATE 66
TI ***Structure*** - ***function*** studies of [2Fe-2S] ferredoxins.

L9 ANSWER 145 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI Structure and dynamics of the neutrophil defensins NP-2, NP-5, and HNP-1: ***NMR*** studies of amide hydrogen exchange kinetics.

L9 ANSWER 146 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Solution structure of RP 71955, a new 21 amino acid tricyclic ***peptide*** active against HIV-1 virus

L9 ANSWER 147 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Function*** and ***three*** - ***dimensional*** ***structure*** of ***proteins*** using ***nuclear*** ***magnetic*** ***resonance*** spectroscopy

L9 ANSWER 148 OF 189 MEDLINE DUPLICATE 67
TI Primary and ***three*** - ***dimensional*** structure of lactotransferrin (lactoferrin) glycans.

L9 ANSWER 149 OF 189 TOXLINE
TI ***STRUCTURE*** - ***FUNCTION*** STUDY OF COBRATOXIN.

L9 ANSWER 150 OF 189 MEDLINE DUPLICATE 68
TI Solution structure of a complex between [N-MeCys3,N-MeCys7]TANDEM and [d(GATATC)]2.

L9 ANSWER 151 OF 189 MEDLINE DUPLICATE 69
TI The role of asparagine-32 in forming the receptor-binding epitope of human epidermal growth factor.

L9 ANSWER 152 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 70
TI The use of osmolytes to facilitate ***protein*** ***NMR*** spectroscopy.

L9 ANSWER 153 OF 189 MEDLINE
TI ***Structure*** and ***function*** of phosphatidylinositol 3-kinase: a potential second messenger system involved in growth control.

L9 ANSWER 154 OF 189 MEDLINE DUPLICATE 71
TI An automated method for modeling ***proteins*** on known templates using distance geometry.

L9 ANSWER 155 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI The use of synthetic ***peptides*** to unravel the mechanism of muscle regulation.

L9 ANSWER 156 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Folding topology and DNA binding of the N-terminal fragment of Ada ***protein***

L9 ANSWER 157 OF 189 TOXLINE
TI CHEMICAL/IMMUNOCHEMICAL STUDIES OF MYOTOXIC ***PROTEINS*** .

L9 ANSWER 158 OF 189 TOXLINE
TI ***STRUCTURE*** - ***FUNCTION*** STUDIES ON MICROSOMAL MEMBRANES.

L9 ANSWER 159 OF 189 MEDLINE DUPLICATE 72
TI Selenomethionyl dihydrofolate reductase from Escherichia coli. Comparative biochemistry and 77Se ***nuclear*** ***magnetic*** ***resonance*** spectroscopy.

L9 ANSWER 160 OF 189 MEDLINE DUPLICATE 73
TI Induced ***peptide*** conformations in different antibody complexes: molecular modeling of the ***three*** - ***dimensional*** structure of ***peptide*** -antibody complexes using ***NMR*** -derived distance restraints.

L9 ANSWER 161 OF 189 MEDLINE
TI Inhibition of cellular proliferation by ***peptide*** analogues of insulin-like growth factor 1.

L9 ANSWER 162 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 74
TI SECONDARY STRUCTURE AND TOPOLOGY OF INTERLEUKIN-1 RECEPTOR ANTAGONIST
PROTEIN DETERMINED BY HETERONUCLEAR ***THREE*** - ***DIMENSIONAL*** ***NMR*** SPECTROSCOPY.

L9 ANSWER 163 OF 189 MEDLINE DUPLICATE 75
TI Mutations at the dimer, hexamer, and receptor-binding surfaces of insulin independently affect insulin-insulin and insulin-receptor interactions.

L9 ANSWER 164 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI SOLUTION STUDIES OF STAPHYLOCOCCAL NUCLEASE H124L 2 PROTON CARBON-13 AND
NITROGEN-15 CHEMICAL SHIFT ASSIGNMENTS FOR THE UNLIGATED ENZYME AND
ANALYSIS OF CHEMICAL SHIFT CHANGES THAT ACCOMPANY FORMATION OF THE
NUCLEASE THYMIDINE 3' 5'-BISPHOSPHATE-CALCIUM TERNARY COMPLEX.

L9 ANSWER 165 OF 189 MEDLINE DUPLICATE 76
TI Characterization of the bacterially expressed Drosophila engrailed homeodomain.

L9 ANSWER 166 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.
TI RNase H: ***Three*** - ***dimensional*** ***structure*** and ***function*** .

L9 ANSWER 167 OF 189 MEDLINE DUPLICATE 77
TI ***Structure*** - ***function*** relationships in human epidermal growth factor studied by site-directed mutagenesis and 1H ***NMR*** .

L9 ANSWER 168 OF 189 MEDLINE DUPLICATE 78
TI ***Structure*** and ***structure*** - ***function*** relationships of sea anemone ***proteins*** that interact with the sodium channel.

L9 ANSWER 169 OF 189 MEDLINE
TI ***Protein*** crystal growth in microgravity.

L9 ANSWER 170 OF 189 MEDLINE DUPLICATE 79
TI Folding and ***activity*** of hybrid sequence, disulfide-stabilized ***peptides*** .

L9 ANSWER 171 OF 189 MEDLINE DUPLICATE 80
TI The structure of the homeodomain and its functional implications.

L9 ANSWER 172 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Determination of ***protein*** structure in aqueous solution with and without distance constraints

L9 ANSWER 173 OF 189 MEDLINE
TI ***Proteins*** as biological effectors.

L9 ANSWER 174 OF 189 MEDLINE DUPLICATE 81
TI Conformational characterization of a single-site mutant of murine epidermal growth factor (EGF) by 1H ***NMR*** provides evidence that leucine-47 is involved in the interactions with the EGF receptor.

L9 ANSWER 175 OF 189 MEDLINE
TI ***Three*** - ***dimensional*** ***structure*** and ***function*** of epidermal growth factor.

L9 ANSWER 176 OF 189 MEDLINE DUPLICATE 82
TI Enzymatic approaches to probing of RNA secondary and ***tertiary*** ***structure*** .

L9 ANSWER 177 OF 189 MEDLINE
TI ***Tertiary*** ***structure*** of human complement component C5a in solution from ***nuclear*** ***magnetic*** ***resonance*** data.

L9 ANSWER 178 OF 189 LIFESCI COPYRIGHT 1999 CSA
TI ***Structure*** and ***function*** of ***proteins*** .

L9 ANSWER 179 OF 189 MEDLINE DUPLICATE 83
TI ***Structure*** - ***function*** relationship in Escherichia coli translational initiation factors. Characterization of IF1 by high-resolution 1H- ***NMR*** spectroscopy.

L9 ANSWER 180 OF 189 MEDLINE DUPLICATE 84
TI Quaternary ***structure*** and ***function*** in phage lambda repressor: 1H- ***NMR*** studies of genetically altered ***proteins*** .

L9 ANSWER 181 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI Characterization of specific fluorenylmethyloxycarbonyl-containing calmodulin adducts by spectroscopy and phosphodiesterase stimulation

L9 ANSWER 182 OF 189 MEDLINE DUPLICATE 85
TI ***Structure*** and ***function*** of the proline-rich region of myelin basic ***protein*** .

L9 ANSWER 183 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
TI ANNUAL REVIEW OF BIOPHYSICS AND BIOENGINEERING VOL. 13 1984.

L9 ANSWER 184 OF 189 MEDLINE DUPLICATE 86
TI ***Structure*** - ***function*** relationship in Escherichia coli translational initiation factors. Characterization of IF-3 by high resolution 1H ***NMR*** spectroscopy.

L9 ANSWER 185 OF 189 CAPLUS COPYRIGHT 1999 ACS
TI ***Structure*** - ***function*** relationship in Escherichia coli initiation factors: VII. Biochemical and proton ***NMR*** spectroscopic study on the involvement of the His residue in the interaction between IF3 and ribosomes

L9 ANSWER 186 OF 189 MEDLINE
TI Physical chemical studies of the ***structure*** and ***function*** of DNA binding (helix-destabilizing) ***proteins*** .

L9 ANSWER 187 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE
TI Computational tools for experimental determination and theoretical prediction of protein structure.

L9 ANSWER 188 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE
TI Workshop on high-field NMR and biological applications.

L9 ANSWER 189 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE
TI Development of experimental techniques to study protein and nucleic acid structures.

=> d 2,17,34,37,40,71,96,106,120,125,147,154,187 bib ab

L9 ANSWER 2 OF 189 CAPLUS COPYRIGHT 1999 ACS
AN 1999:303259 CAPLUS
DN 130:308199
TI Linking gene sequence to gene ***function*** by ***three*** - ***dimensional*** ***protein*** ***structure*** determination using ***NMR***
IN Anderson, Stephen; Montelione, Gaetano
PA Rutgers, the State University of New Jersey, USA
SO PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9922019	A1	19990506	WO 1998-US22839	19981029

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI US 1997-63679 19971029
US 1998-181601 19981029
AB The present invention provides a ***structure*** - ***functional*** anal. engine for the high-throughput detn. of the biochem. ***function*** of ***proteins*** or ***protein*** domains of unknown ***function*** . The present invention uses bioinformatics, mol. biol. and ***NMR*** tools for the rapid and automated detn. of the ***three*** - ***dimensional*** structures of ***proteins*** and ***protein*** domains.

L9 ANSWER 17 OF 189 CAPLUS COPYRIGHT 1999 ACS
AN 1999:146268 CAPLUS
TI ***Protein*** ***NMR*** and the human proteome project
AU Montelione, Gaetano T.
CS Center for Advanced Biotechnology Medicine and Department of Molecular Biology and Biochemistry, Rutgers University, Piscataway, NJ, 08854, USA
SO Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25 (1999), POLY-232 Publisher: American Chemical Society, Washington, D. C.
CODEN: 67GHA6
DT Conference; Meeting Abstract
LA English
AB Genome sequencing projects are rapidly identifying all of the genes in several organisms. The products of these genes are widely recognized as the next generation of therapeutics and targets for the development of pharmaceuticals. While identification of these genes is proceeding quickly, elucidation of their ***three*** ***dimensional*** (3D) ***structures*** and biochem. ***functions*** lags far behind. In some cases, knowledge of 3D structures of ***proteins*** can provide important insights into structural homol. that is not easily recognized by sequence alignment comparisons. Thus, anal. of a ***protein*** 's 3D structure by ***NMR*** or X-ray crystallog. prior to characterization of the ***protein*** 's biochem. ***function*** can sometimes provide key information regarding ***protein*** fold class, locations and clustering of conserved residues, and surface electrostatic field distributions. This information can be used to develop hypotheses regarding potential biochem. functions, and the resulting limited set of putative biochem. functions tested by appropriate biochem. assays. ***NMR*** chem. shift assignments and soln. structures of ***proteins*** also provide the basis for epitope-mapping, mol. dynamics, and SAR studies, and set the stage for subsequent drug development using combinatorial and/or rational design methods. We are developing technologies that will significantly accelerate the process of structure detn. by ***NMR*** . These include bioinformatics methods for parsing novel genes into domain encoding regions, high-level "multiplexed" ***protein*** expression systems, and ***NMR*** pulse sequences, data collection methods, and expert-system software for automated anal. of ***protein*** resonance assignments and 3D structures. These technologies and the resulting exptl. data are being organized and integrated using relational databases. The goal of this work is to develop a "high-throughput" process for structural anal. of novel gene products on a genomic scale. In a pilot project, these techniques are being applied to clusters of orthologous genes coding for ***proteins*** of unknown ***structure*** and ***function*** , with the aim of testing the hypothesis that 3D structural anal. can sometimes provide useful and important clues regarding the biochem. functions of orphan gene products. The relationship of our effort and the emerging international interest in a large-scale Human Proteome Project will be discussed.

L9 ANSWER 34 OF 189 MEDLINE DUPLICATE 17
AN 1998387899 MEDLINE
DN 98387899
TI Method for prediction of ***protein*** ***function*** from sequence using the sequence-to- ***structure*** -to- ***function*** paradigm with application to glutaredoxins/thioredoxins and T1 ribonucleases.
AU Fetrow J S; Skolnick J
CS Center for Biochemistry and Biophysics, University at Albany, SUNY, 1400 Washington Avenue, Albany, NY 12222, USA.
SO JOURNAL OF MOLECULAR BIOLOGY, (1998 Sep 4) 281 (5) 949-68. Journal code: J6V. ISSN: 0022-2836.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals; Cancer Journals
EM 199812
EW 19981202
AB The practical exploitation of the vast numbers of sequences in the genome sequence databases is crucially dependent on the ability to identify the ***function*** of each sequence. Unfortunately, current methods, including global sequence alignment and local sequence motif identification, are limited by the extent of sequence similarity between sequences of unknown and known ***function*** ; these methods

increasingly fail as the sequence identity diverges into and beyond the twilight zone of sequence identity. To address this problem, a novel method for identification of ***protein*** ***function*** based directly on the sequence-to- ***structure*** -to- ***function*** paradigm is described. Descriptors of ***protein*** active sites, termed "fuzzy functional forms" or FFFs, are created based on the geometry and conformation of the active site. By way of illustration, the active sites responsible for the disulfide oxidoreductase ***activity*** of the glutaredoxin/thioredoxin family and the RNA hydrolytic ***activity*** of the T1 ribonuclease family are presented. First, the FFFs are shown to correctly identify their corresponding active sites in a library of exact ***protein*** models produced by crystallography or ***NMR*** spectroscopy, most of which lack the specified ***activity*** . Next, these FFFs are used to screen for active sites in low-to-moderate resolution models produced by ab initio folding or threading prediction algorithms. Again, the FFFs can specifically identify the functional sites of these ***proteins*** from their predicted structures. The results demonstrate that low-to-moderate resolution models as produced by state-of-the-art ***tertiary*** ***structure*** prediction algorithms are sufficient to identify ***protein*** active sites. Prediction of a novel ***function*** for the gamma subunit of a yeast glycosyl transferase and prediction of the ***function*** of two hypothetical yeast ***proteins*** whose models were produced via threading are presented. This work suggests a means for the large-scale functional screening of genomic sequence databases based on the prediction of structure from sequence, then on the identification of functional active sites in the predicted structure. Copyright 1998 Academic Press

L9 ANSWER 37 OF 189 MEDLINE
AN 1998290966 MEDLINE
DN 98290966
TI Recent trends in ***protein*** structural studies.
AU Titani K; Hayashi N
CS Division of Biomedical Polymer Science, Institute for Comprehensive Medical Science, Fujita Health University, Toyoake.
SO RINSHO BYORI. JAPANESE JOURNAL OF CLINICAL PATHOLOGY, (1998 May) 46 (5)
450-5. Ref: 0
Journal code: KIV. ISSN: 0047-1860.
CY Japan
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW LITERATURE)
LA Japanese
EM 199810
EW 19981005
AB Since the 1980's, structural studies of ***proteins*** have changed remarkably. It is currently possible to predict the entire amino acid sequence of a ***protein*** by the rapid and highly sensitive analysis of the nucleotide sequence of genomic DNA or cDNA encoding the ***protein*** . In the near future, the entire sequence of a ***protein*** may be predicted from a partial sequence just by searching a variety of databases now being constructed for many biological species. The predicted ***protein*** sequence, however, is the backbone structure of the precursor ***protein*** without post-translational modifications. Therefore, the major objectives of recent structural studies of ***proteins*** are directed to 1) rapid and sensitive confirmation of the predicted sequence and identification of those modifications present in mature ***proteins*** by newly developed mass spectrometry, 2) determination of the 3D structures of intact and mutant ***proteins*** isolated or expressed in cultured E. coli, yeast or animal cells using X-ray crystallography or ***NMR*** analysis, and 3) rapid prediction of the 3D structures of ***proteins*** utilizing ***protein*** databases. The "PROTEOME" project was proposed in 1998 to bring together all the data on the ***structure*** and ***function*** of mature ***proteins*** under international cooperation. The present paper summarizes such recent trends in ***protein*** structural studies.

L9 ANSWER 40 OF 189 CAPLUS COPYRIGHT 1999 ACS
AN 1998:328663 CAPLUS
DN 129:133145
TI The development of ***NMR*** methods to study ***protein*** structure and dynamics
AU Kay, Lewis E.
CS Departments of Medical Genetics, Biochemistry and Chemistry, University of Toronto, Toronto, ON, M5S 1A8, Can.
SO NATO ASI Ser., Ser. C (1998), 510(New Methods for the Study of Biomolecular Complexes), 285-293
CODEN: NSCSDW; ISSN: 0258-2023
PB Kluwer Academic Publishers
DT Journal; General Review
LA English
AB A review with 28 refs. An understanding of the role played by a ***protein*** in cellular ***function*** requires a detailed picture of its ***three*** - ***dimensional*** structure as well as an appreciation of how the ***structure*** varies as a ***function*** of time due to mol. dynamics. Over the past several years multi-dimensional, multi-nuclear soln. ***NMR*** spectroscopy has become a powerful technol. for obtaining both structural and dynamic information on ***proteins*** and ***protein*** -ligand systems. However, until recently the methods were limited to the study of mols. having mol. wts. on the order of 25 kDa or less. Recent developments making use of fractional or complete deuteration have increased the scope of structural studies by ***NMR*** and have also improved studies of

L9 ANSWER 71 OF 189 MEDLINE DUPLICATE 36
AN 1998046743 MEDLINE
DN 98046743
TI TESS: a geometric hashing algorithm for deriving 3D coordinate templates for searching structural databases. Application to enzyme active sites.
AU Wallace A C; Borkakoti N; Thornton J M
CS Department of Biochemistry and Molecular Biology, University College, London, England.
SO PROTEIN SCIENCE, (1997 Nov) 6 (11) 2308-23.
Journal code: BNW. ISSN: 0961-8368.
EM 199804
EW 19980403
AB It is well established that sequence templates such as those in the PROSITE and PRINTS databases are powerful tools for predicting the biological ***function*** and ***tertiary*** ***structure*** for newly derived ***protein*** sequences. The number of X-ray and ***NMR*** ***protein*** structures is increasing rapidly and it is apparent that a 3D equivalent of the sequence templates is needed. Here, we describe an algorithm called TESS that automatically derives 3D templates from structures deposited in the Brookhaven ***Protein*** Data Bank. While a new sequence can be searched for sequence patterns, a new structure can be scanned against these 3D templates to identify functional sites. As examples, 3D templates are derived for enzymes with an O-His-O "catalytic triad" and for the ribonucleases and lysozymes. When these 3D templates are applied to a large data set of nonidentical ***proteins*** , several interesting hits are located. This suggests that the development of a 3D template database may help to identify the ***function*** of new ***protein*** ***structures*** , if unknown, as well as to design ***proteins*** with specific functions.

L9 ANSWER 96 OF 189 MEDLINE DUPLICATE 52
AN 97120677 MEDLINE
DN 97120677
TI What ***function*** for human lithostathine?: structural investigations by ***three*** - ***dimensional*** structure modeling and high-resolution ***NMR*** spectroscopy.
AU Patard L; Stoven V; Gharib B; Bontems F; Lallemand J Y; De Reggi M
CS Laboratoire de RMN, URA 1308 du CNRS, DCSO, Ecole Polytechnique, Palaiseau, France.
SO PROTEIN ENGINEERING, (1996 Nov) 9 (11) 949-57.
Journal code: PRI. ISSN: 0269-2139.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199705
EW 19970504
AB Human lithostathine is a 144-residue ***protein*** , expressed in various organs and pathologies. Several biological functions have been proposed for this ***protein*** . Among others, inhibition of nucleation and growth of CaCO3 crystals in the pancreas and bacterial aggregation has retained attention, because lithostathine presents high sequence similarities with calcium-dependent (or C-type) lectins. To study its ***structure*** - ***function*** relationship and compare it with that of C-type lectins, we have built a model for lithostathine. This model is derived from the only two C-type lectins of known structures: rat mannose binding ***protein*** and human E-selectin. An original strategy, inspired by that proposed by Havel and Snow, was designed for model building. We have undertaken ***NMR*** studies on the natural ***protein*** . Although complete structure determination has not yet been achieved, the ***NMR*** studies did confirm the main characteristics of the model. From analysis of the proposed model, we concluded that lithostathine is not expected to present sugar- or calcium-binding properties. Therefore, the mechanisms of bacterial aggregation and inhibition of CaCO3 nucleation and growth have not yet been elucidated.

L9 ANSWER 106 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 56
AN 1996:202695 CAPLUS
DN 124:253414
TI Modern ***NMR*** spectroscopy and x-ray crystallography. Different approaches to study the ***structure*** and its ***function*** of a ***protein***
AU Tsuda, Sakae
CS Biosci. Chem. Div., Hokkaido Natl. Ind. Res. Inst., Sapporo, 062, Japan
SO Nippon Kessho Gakkaishi (1996), 38(1), 84-8
CODEN: NKEGAF; ISSN: 0369-4585
DT Journal; General Review
LA Japanese
AB A review with 27 refs. The ***NMR*** spectroscopy has been utilized widely for a elucidation of the structural changes of ***proteins*** caused by changes in pH, ionic strength, temp., and ligand concn. in soln. The x-ray was less utilized for these studies executable easily in soln., but is utilized much for the structural detn. of a ***protein*** .

Such difference has lead to the situation where the ***NMR*** relied on the structure solved by x-ray and the x-ray argued its structure in ref. to the conformational change elucidated by ***NMR*** . However, recent developments of ***NMR*** spectroscopy made it possible to det. the ***three*** - ***dimensional*** structure, and x-ray techniques has also been developed to clarify the structural changes of a ***protein*** . This review compares the recent development of these two techniques, and will discuss about the future collaborating interaction between ***NMR*** and x-ray.

L9 ANSWER 120 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS
AN 1995:309145 BIOSIS
DN PREV199598323445
TI ***NMR*** : This other method for ***protein*** and nucleic acid structure determination.
AU Wuthrich, Kurt
CS Inst. Molekularbiol. und Biophysik, Eidgenossische Technische Hochschule-Honggerberg, CH-8093 Zurich Switzerland
SO Acta Crystallographica Section D Biological Crystallography, (1995) Vol. 51, No. 3, pp. 249-270.
ISSN: 0907-4449.
AB For a quarter of a century X-ray diffraction in single crystals was unique in its ability to solve ***three*** - ***dimensional*** structures of ***proteins*** and nucleic acids at atomic resolution. The situation changed in 1984 with the completion of a ***protein*** structure determination by ***nuclear*** ***magnetic*** ***resonance*** (***NMR***) spectroscopy in solution, and today ***NMR*** is a second widely used method for biomacromolecular structure determination. This review describes the method of ***NMR*** structure determination of biological macromolecules, and attempts to place ***NMR*** structure determination in perspective with X-ray crystallography. ***NMR*** is most powerful for studies of relatively small systems with molecular weights up to about 30000, but these structures can be obtained in near-physiological milieus. The two techniques have widely different time scales which afford different insights into internal molecular mobility as well as different views of ***protein*** or nucleic acid molecular surfaces and hydration. Generally, in addition to information on the average ***three*** - ***dimensional*** structure, ***NMR*** provides information on a wide array of short-lived transient conformational states. Combining information from the two methods can yield a more detailed insight into the structural basis of ***protein*** and nucleic acid functions, and thus provide a more reliable platform for rational drug design and the engineering of novel ***protein*** functions.

L9 ANSWER 125 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 62
AN 1995:774534 CAPLUS
DN 123:163615
TI ***Structure*** and ***function*** of ***protein*** modules
AU Go, Mitiko
CS Toyota Phys. Chem. Res. Inst., Aichi, 480-11, Japan
SO Toyota Kenkyu Hokoku (1995), 48, 81-5
CODEN: TOKHA6; ISSN: 0372-039X
LA Japanese
AB Globular ***proteins*** are decompd. into several compact modules. Modules consist of about 10-40 contiguous amino acid residues and module boundaries are correlated with intron positions of genes. To clarify physico-chem. basis of modules as structural units of ***proteins*** , the authors synthesized module M1 of barnase, a bacterial RNase, and detd. its secondary structure in soln. by using ***NMR*** technique. M1 had an .alpha.-helix at the similar location to the corresponding helix of the intact barnase. This result shows that the excised module has propensity to form similar secondary structure to those of the intact barnase. This propensity should be an important feature of modules advantageous as parts recruited into globular ***proteins*** through exon shuffling in early evolution. To identify functionally important regions of large ***proteins*** without their ***three*** - ***dimensional*** information, the authors applied a method for prediction of module boundaries to human CCG1. The authors obtained a close correlation between predicted modules and exon/intron structure of human CCG1 gene. Predicted 152 modules of CCG1 show a close correlation with temporary assigned ***function*** of CCG1. This result opens a new exptl. approach to det. functionally important regions of huge ***proteins*** ; synthesis of a module or jointed modules of the ***proteins*** by chem. method and detn. of its ***function*** will be useful for identification of each functional region of ***proteins*** .

L9 ANSWER 147 OF 189 CAPLUS COPYRIGHT 1999 ACS
AN 1995:473516 CAPLUS
DN 122:234586
TI ***Function*** and ***three*** - ***dimensional*** ***structure*** of ***proteins*** using ***nuclear*** ***magnetic*** ***resonance*** spectroscopy
AU Poulsen, Flemming M.
CS Kemisk Afdeling, Carlsberg Laboratorium, Copenhagen, DK-2500, Den.
SO Protein Struct. Distance Anal. (1994), 24-35, 2 plate. Editor(s): Bohr, Henrik; Brunak, Soeren. Publisher: IOS Press, Amsterdam, Neth.
CODEN: 61CIAF
DT Conference
LA English
AB Although the ***three*** - ***dimensional*** structure of a ***protein*** can provide valuable information and stimulate rational investigation of other important features of the ***protein*** it is important to stress that a structure per se is rarely a revelation of the biol. ***function*** of the ***protein*** . This paper emphasizes the importance of acquiring results that measure the fundamental phys. chem. parameters in ***protein*** ***function*** events and the importance of getting quant. information to support our understanding of the link between phys. parameters that describe ***function*** and the biol. relevance of a ***protein*** mol. It is emphasized that ***NMR*** spectroscopy, because it combines the ability of measuring ***three*** - ***dimensional*** structure and the ability of measuring many phys. parameters related to both ***structure*** and ***function*** , is one of the key techniques in structural biol.

L9 ANSWER 154 OF 189 MEDLINE DUPLICATE 71
AN 93184745 MEDLINE
DN 93184745
TI An automated method for modeling ***proteins*** on known templates using distance geometry.
AU Srinivasan S; March C J; Sudarsanam S
CS Department of Protein Chemistry, Immunex Corporation, Seattle, Washington 98101..
SO PROTEIN SCIENCE, (1993 Feb) 2 (2) 277-89.
Journal code: BNW. ISSN: 0961-8368.
AB We present an automated method incorporated into a software package, FOLDER, to fold a ***protein*** sequence on a given ***three*** - ***dimensional*** (3D) template. Starting with the sequence alignment of a family of homologous ***proteins*** , tertiary structures are modeled using the known 3D structure of one member of the family as a template. Homologous interatomic distances from the template are used as constraints. For nonhomologous regions in the model ***protein*** , the lower and the upper bounds for the interatomic distances are imposed by steric constraints and the globular dimensions of the template, respectively. Distance geometry is used to embed an ensemble of structures consistent with these distance bounds. Structures are selected from this ensemble based on minimal distance error criteria, after a penalty ***function*** optimization step. These ***structures*** are then refined using energy optimization methods. The method is tested by simulating the alpha-chain of horse hemoglobin using the alpha-chain of human hemoglobin as the template and by comparing the generated models with the crystal structure of the alpha-chain of horse hemoglobin. We also test the packing efficiency of this method by reconstructing the atomic positions of the interior side chains beyond C beta atoms of a ***protein*** domain from a known 3D structure. In both test cases, models retain the template constraints and any additionally imposed constraints while the packing of the interior residues is optimized with no short contacts or bond deformations. To demonstrate the use of this method in simulating structures of ***proteins*** with nonhomologous disulfides, we construct a model of murine interleukin (IL)-4 using the ***NMR*** structure of human IL-4 as the template. The resulting geometry of the nonhomologous disulfide in the model structure for murine IL-4 is consistent with standard disulfide geometry.

L9 ANSWER 187 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE
AN 1996(21):152509 ENERGY
TI Computational tools for experimental determination and theoretical prediction of protein structure.
AU O'Donoghue, S.; Rost, B.
CS Stanford Univ., CA (United States)
Funding Organisation: USDOE, Washington, DC (United States)
NC FG03-95ER62031
NR CONF-9507246--3
SO [1995]. 156 p. OSTI as DE96014300; NTIS; US Govt. Printing Office Dep.
Conference: Intelligent Systems for Molecular Biology (ISMB) conference, Cambridge (United Kingdom), 16-19 Jul 1995
AB This tutorial was one of eight tutorials selected to be presented at the Third International Conference on Intelligent Systems for Molecular Biology which was held in the United Kingdom from July 16 to 19, 1995. The authors intend to review the state of the art in the experimental determination of protein 3D structure (focus on nuclear magnetic resonance), and in the theoretical prediction of protein function and of protein structure in 1D, 2D and 3D from sequence. All the atomic resolution structures determined so far have been derived from either X-ray crystallography (the majority so far) or Nuclear Magnetic Resonance (NMR) Spectroscopy (becoming increasingly more important). The authors briefly describe the physical methods behind both of these techniques; the major computational methods involved will be covered in some detail. They highlight parallels and differences between the methods, and also the current limitations. Special emphasis will be given to techniques which have application to ab initio structure prediction. Large scale sequencing techniques increase the gap between the number of known proteins sequences and that of known protein structures. They describe the scope and principles of methods that contribute successfully to closing that gap. Emphasis will be given on the specification of adequate testing procedures to validate such methods